

Renormalization of transition matrix elements of particle number operators due to strong electron correlation

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Abstract. Renormalization of non-magnetic and magnetic impurities due to electron double occupancy prohibition is derived analytically by an improved Gutzwiller approximation. Non-magnetic impurities are effectively weakened by the same renormalization factor as that for the hopping amplitude, whereas magnetic impurities are strengthened by the square root of the spin-exchange renormalization factor, in contrast to results by the conventional Gutzwiller approximation. We demonstrate it by showing that transition matrix elements of number operators between assumed excited states and between an assumed ground state and excited states are renormalized differently than diagonal matrix elements. Deviation from such simple renormalization with a factor is also discussed. In addition, as related calculation, we correct an error in treatment of renormalization of charge interaction in the literature. Namely, terms from the second order of the transition matrix elements are strongly suppressed. Since all these results do not depend on the signs of impurity potential or charge interaction parameter, they are valid both in attractive and repulsive cases.

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1. Introduction

In this paper, we discuss renormalization of impurities due to strong electron correlation. Such renormalization may be intuitive in the case of the Hubbard model, where each site has onsite electron repulsion. Namely, sites with higher potential energy have lower electron occupancy, and consequently have less chance of double occupancy. Then, the total energy loss from the impurity potential and the repulsive interaction should be more uniform than in the system without the electron correlation; we can call it renormalization of impurities. However, when the repulsion is very strong, we need to consider much smaller energy scales. That is, if double occupancy does not occur, the above argument cannot be applied, and thus renormalization of impurities within the lower Hubbard band is not so trivial.

When electron double occupancy is prohibited at every site, a system with quite densely packed electrons has a good chance to have one electron with spin up or down at each site. If the system has a tendency toward phase separation, small perturbation by an impurity may produce a large effect to separate a system into hole-rich regions and electron-rich regions; it may appear in close vicinity of the half filling in the t - J -type models, where effective hopping is negligibly small compared to effective exchange interaction. In contrast, what we focus on in this paper are systems not that close to the half filling or systems with relatively weak exchange interaction. Then, electrons are more mobile. Near the half filling, since there is little freedom left to change charge distribution and sudden spatial change of particle number distribution around impurities is not favorable for the kinetic energy, non-magnetic impurity potentials may have little effect on low-energy eigenstates and only shift their eigenenergies quite uniformly. In other words, impurity potentials can be renormalized by electron correlation even within the lower Hubbard band.

In previous papers [1, 2], such renormalization of non-magnetic impurity potentials was investigated numerically. That is, (i) to estimate perturbation from an impurity potential, the variational Monte Carlo method was applied to calculation of its matrix elements with respect to assumed excited states in the uniform systems; (ii) inhomogeneous systems with an impurity or impurities were investigated by a Bogoliubov-de Gennes equation with the double-occupancy prohibition treated by a kind of mean-field approximation called the Gutzwiller approximation (GA) generalized to inhomogeneous systems.

Both of (i) and (ii) manifested strong renormalization of the impurity potential, and its renormalization factor (ratio between corresponding quantities in systems with and without the double-occupancy prohibition) seems approximately proportional to $g^t \equiv 2x/(1+x)$, which is the renormalization factor of hopping amplitude obtained by the GA as a function of hole concentration x . Since the double-occupancy prohibition inhibits hopping, g^t is less than unity and goes to zero as $x \rightarrow 0$. To explain the impurity renormalization factor close to g^t , we pointed out the similarity between the impurity potential and the hopping in the real space, i.e., the Fourier-transformed impurity

potential has the form of hopping in the k -space. If electrons are densely packed in the lattice, it must be difficult even in the k -space to hop from k to a different k' .

However, it is a speculation and may not be trivial because the double occupancy is prohibited in the real space rather than in the k -space. In addition, we do not really know how general the numerical results are because the calculation was done only for limited parameter sets. To complement this argument, an analytic approximation is adopted in this paper, namely, (i) is redone using the GA to derive dominant g^t dependence and deviation from g^t explicitly. In fact, however, the conventional GA [3, 4] fails to derive this renormalization. It compares mean weights of configurations relevant to operators of interest with and without the electron repulsion in calculating the renormalization factors. Then, the renormalization factor for the particle number operators is actually unity, i.e., they are not renormalized. The spin rotation invariant slave-boson mean-field theory [5] is known to be equivalent to the conventional GA; the saddle-point approximated boson fields play a role of the weights in the GA. Therefore, we speculate that it may have the same problem as the conventional GA. In addition, we believe that the slave-boson mean-field theory with only one boson often used for the t - J model can be even less accurate because it does not yield renormalization of the exchange interaction, which may be an artifact from the lost boson hard-core property.

Let us recall that the GA corresponds to taking the leading order of the Wick expansion with respect to the intersite contractions of creation/annihilation operators [6, 7]. In fact, the weights of configurations in the conventional GA are likely to be calculated with the focus only on the lowest order; apparently it breaks down when the lowest order vanishes or when the next lowest order is of interest. An example is a particle number operator as shown in this paper. Although the lowest order is the average particle number, when we discuss transition matrix elements with excited states, this lowest order does not contribute, and the next lowest order is relevant. We will demonstrate that off-diagonal matrix elements between an assumed ground state and excited states as well as between different excited states are renormalized differently than diagonal matrix elements.

Furthermore, by slightly modifying the non-magnetic impurity, i.e., by subtraction between up- and down-spin particle number operators, we also consider a simple magnetic impurity. In this case, the direction of the renormalization is reversed, namely, the impurity is strengthened by the electron correlation in contrast to the non-magnetic impurity. It must be physically reasonable because electron repulsion increases single occupancy. As calculation related to the non-magnetic impurity, renormalization of charge interaction is discussed to correct an error in its treatment in the literature. That is, terms relevant to the mean-field approximation are actually the second order of the transition matrix elements, and they are weakened by very small renormalization factor $(g^t)^2$ although treated usually as not being renormalized.

2. Model

What we have in mind is t - J -type models with impurities, namely,

$$H \equiv P_G \left[- \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,j} J_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j \right) + H_{\text{imp}} \right] P_G, \quad (1)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is the creation (annihilation) operator of the electron with site i and spin σ , and \mathbf{S}_i is the spin operator at site i . In addition,

$$\hat{n}_i \equiv \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}, \quad \hat{n}_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}. \quad (2)$$

Gutzwiller projection operator $P_G \equiv \prod_i (1 - \hat{n}_{i\uparrow} \hat{n}_{i\downarrow})$ prohibits electron double occupancy at each site and represents strong Coulomb repulsion. In this paper, we do not use any explicit form of t_{ij} and J_{ij} although they are implicitly included in assumed variational ground/excited states. Our main focus here is on the impurity term H_{imp} .

In sections 3, 4 and 5, our target is renormalization of a single non-magnetic δ -function impurity potential located at $i = I$,

$$H_{\text{imp}} = V_I \hat{n}_I = V_I (\hat{n}_{I\uparrow} + \hat{n}_{I\downarrow}). \quad (3)$$

Then, in section 6, we discuss renormalization of a simple magnetic impurity,

$$H_{\text{imp}} = -h_I S_I^z = -\frac{h_I}{2} (\hat{n}_{I\uparrow} - \hat{n}_{I\downarrow}). \quad (4)$$

In addition, the focus in section 7 is not on H_{imp} but on charge interaction $\hat{n}_i \hat{n}_j$ in Hamiltonian (1).

3. Non-magnetic impurity renormalization

Let us start from a uniform system without impurities. A basic idea of variational theories is that the ground state of the t - J -type models may be something similar to the BCS superconducting state

$$|\Psi_0\rangle \equiv \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |0\rangle, \quad (5)$$

but somewhat modified by the electron correlation. Simple variational wave functions adopted by most of analytic theories have a form of $P_G |\Psi_0\rangle$ with something to control the particle number. One way to control it is to use projection P_N to fixed particle number N .[‡] Another is to attach fugacity factors to the projector, namely,

$$|\Psi\rangle \equiv P |\Psi_0\rangle, \quad P \equiv \prod_i P_i, \quad P_i \equiv \lambda_{i\uparrow}^{\frac{1}{2}\hat{n}_{i\uparrow}} \lambda_{i\downarrow}^{\frac{1}{2}\hat{n}_{i\downarrow}} (1 - \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}). \quad (6)$$

The latter is adopted in this paper. The reason to control the particle number is that P_G changes the average particle number of $|\Psi_0\rangle$ because states with a larger particle

[‡] Many different $|\Psi_0\rangle$ correspond to $|\Psi\rangle$ under the projections. For example, $\exp(\lambda \hat{N})$ with \hat{N} the total particle number operator is constant under P_N , and thus $\exp(\lambda \hat{N}) |\Psi_0\rangle$ is equivalent to $|\Psi_0\rangle$.

number have more chance to be projected out [8]. Since the GA relates expectation values before and after the projection,

$$\langle \hat{O} \rangle_0 \equiv \langle \Psi_0 | \hat{O} | \Psi_0 \rangle, \quad \langle \hat{O} \rangle \equiv \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad (7)$$

for some operator \hat{O} , usually it is not convenient if $|\Psi\rangle$ and $|\Psi_0\rangle$ are totally different, e.g., if $|\Psi_0\rangle$ has a more-than-half filled electron band. § Although our main interest here is perturbation from the uniform state, most of derivation in this paper is valid also for inhomogeneous systems, and thus we prefer to keep general expressions with site and spin indices throughout the paper, e.g.,

$$n_{i\sigma} \equiv \langle \hat{n}_{i\sigma} \rangle_0, \quad n_i \equiv \langle \hat{n}_i \rangle_0 = n_{i\uparrow} + n_{i\downarrow}. \quad (8)$$

However, we use $0 = \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle_0 = \langle c_{i\sigma}^\dagger c_{j\sigma}^\dagger \rangle_0 = \langle c_{i\uparrow}^\dagger c_{j\downarrow} \rangle_0$ to avoid making formulas too lengthy.

Although choice of the fugacity factors is not unique especially in inhomogeneous systems [7], yet it is convenient to define

$$\lambda_{i\sigma} \equiv \frac{1 - n_{i\sigma}}{1 - n_i}, \quad (9)$$

because it satisfies

$$\langle \hat{n}_{i\sigma} \rangle \approx \langle \hat{n}_{i\sigma} \rangle_0, \quad (10)$$

for any i and σ [6, 7], neglecting terms of the “fourth order”. Here, and throughout this paper, if not specified, “ n -th order” represents n -th order with respect to intersite contractions such as $\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle_0$ and $\langle c_{i\downarrow} c_{j\uparrow} \rangle_0$ with $i \neq j$. Note that $\langle \hat{O} \rangle$ of any \hat{O} can be in principle calculated by the Wick theorem, which yields many such intersite contractions. High order terms may be neglected by recalling that onsite contractions are larger than intersite contractions. The GA corresponds to taking the leading order only, e.g.,

$$\langle P^2 \rangle_0 \approx \prod_i \langle P_i^2 \rangle_0, \quad (11)$$

$$\begin{aligned} \langle P_i^2 \rangle_0 &= (1 - n_{i\uparrow})(1 - n_{i\downarrow}) + \lambda_{i\uparrow} n_{i\uparrow}(1 - n_{i\downarrow}) + \lambda_{i\downarrow} n_{i\downarrow}(1 - n_{i\uparrow}) \\ &= \frac{(1 - n_{i\uparrow})(1 - n_{i\downarrow})}{1 - n_i}. \end{aligned} \quad (12)$$

The terms neglected in the approximation in (11) are of the fourth order because the second order terms cancel out when $\lambda_{i\sigma}$ is defined as (9) [6, 7]. Let us show it explicitly with a notation to treat c^\dagger and c together,

$$c_{i\sigma}^+ \equiv c_{i\sigma}^\dagger, \quad c_{i\sigma}^- \equiv c_{i\sigma}, \quad (13)$$

§ The variational Monte Carlo method does not have such restriction. For example, local magnetic moments before and after the projection are different in general, and the chemical potential in a variational mean-field Hamiltonian is a variational parameter under P_N rather than a parameter to control the particle number.

by considering contractions between P_i^2 and operators at some site(s) $j, j' \neq i$,

$$\begin{aligned} \langle P_i^2 c_{j'\sigma'}^\tau c_{j\sigma}^\tau \rangle_0 &= \langle P_i^2 \rangle_0 \langle c_{j'\sigma'}^\tau c_{j\sigma}^\tau \rangle_0 \\ &+ \left(-\langle c_{i\uparrow} c_{j'\sigma'}^\tau \rangle_0 \langle c_{i\uparrow}^\dagger c_{j\sigma}^\tau \rangle_0 + \langle c_{i\uparrow} c_{j\sigma}^\tau \rangle_0 \langle c_{i\uparrow}^\dagger c_{j'\sigma'}^\tau \rangle_0 \right) [(1 - n_{i\downarrow}) - \lambda_{i\uparrow}(1 - n_{i\downarrow}) + \lambda_{i\downarrow} n_{i\downarrow}] \\ &+ \left(-\langle c_{i\downarrow} c_{j'\sigma'}^\tau \rangle_0 \langle c_{i\downarrow}^\dagger c_{j\sigma}^\tau \rangle_0 + \langle c_{i\downarrow} c_{j\sigma}^\tau \rangle_0 \langle c_{i\downarrow}^\dagger c_{j'\sigma'}^\tau \rangle_0 \right) [(1 - n_{i\uparrow}) + \lambda_{i\uparrow} n_{i\uparrow} - \lambda_{i\downarrow}(1 - n_{i\uparrow})] \end{aligned} \quad (14)$$

for arbitrary τ, τ', σ and σ' . Then, the quantities in the square brackets vanish.

We assume that $|\Psi\rangle$ is a good variational ground state, and that the excited states are well represented by projected quasiparticles

$$|ks\rangle \equiv \frac{P\gamma_{ks}^\dagger |\Psi_0\rangle}{\sqrt{\langle \Psi_0 | \gamma_{ks} P P \gamma_{ks}^\dagger | \Psi_0 \rangle}} \approx \frac{P\gamma_{ks}^\dagger |\Psi_0\rangle}{\sqrt{\langle P^2 \rangle_0}}, \quad (15)$$

where γ_{ks} are quasiparticles for $|\Psi_0\rangle$, namely,

$$\gamma_{k\uparrow}^\dagger = u_k^* c_{k\uparrow}^\dagger - v_k^* c_{-k\downarrow}, \quad \gamma_{-k\downarrow} = v_k c_{k\uparrow}^\dagger + u_k c_{-k\downarrow}. \quad (16)$$

For the denominator of $|ks\rangle$, we have used approximation $\langle \Psi_0 | \gamma_{k\sigma} P^2 \gamma_{k\sigma}^\dagger | \Psi_0 \rangle \approx \langle P^2 \rangle_0$ [7, 9], and errors from this approximation are of the second order.

By switching on the impurity potential, these excited states should be mixed by matrix elements

$$\frac{V_{k',k}}{N_L} \equiv \langle k's | \hat{n}_I | ks \rangle \approx \frac{\langle \gamma_{k's} P \hat{n}_I P \gamma_{ks}^\dagger \rangle_0}{\langle P^2 \rangle_0}, \quad (17)$$

with N_L the number of sites. The limit of the half filling can be exactly evaluated; $\lambda \rightarrow \infty$, $P \hat{n}_I P \rightarrow PP$, and thus $V_{k',k}/N_L \rightarrow \langle k's | ks \rangle = \delta_{k'k}$. According to the BCS theory, $V_{k',k}^{\text{BCS}} \equiv \langle \gamma_{k's} \hat{n}_I \gamma_{ks}^\dagger \rangle_0 = u_{k'} u_k^* - v_{k'} v_k^*$. In the previous paper [2], the author noted that $V_{k',k}$ is not renormalized with the conventional GA [4] because it originally comes from a particle number operator. However, more careful analysis here will show that, although the *diagonal* matrix elements of the particle number operators are not renormalized [eg., see (10)], their *off-diagonal* matrix elements with respect to the projected quasiparticle excited states are renormalized.

The Wick expansion of $\langle \gamma_{k's} P \hat{n}_{I\sigma} P \gamma_{ks}^\dagger \rangle_0$ yields many terms, and some terms contain onsite contraction of $\hat{n}_{I\sigma}$ at the center as $\hat{n}_{I\sigma} \rightarrow n_{I\sigma}$, and the others do not. Let us separate these two groups of terms,

$$\langle \gamma_{k's} P \hat{n}_{I\sigma} P \gamma_{ks}^\dagger \rangle_0 = n_{I\sigma} \langle \gamma_{k's} P^2 \gamma_{ks}^\dagger \rangle_0 + \langle \gamma_{k's} P^2 (\hat{n}_{I\sigma} - n_{I\sigma}) \gamma_{ks}^\dagger \rangle_0. \quad (18)$$

The first term is proportional to $\langle k' \uparrow | k \uparrow \rangle$, and vanishes when $k \neq k'$. Namely, we can only consider the second term.

Let us first take only $\hat{n}_{I\uparrow}$ in the impurity potential term. Since the GA is carried out in the real space, the k representation should be inverse Fourier transformed into the real space representation. Namely, what we should calculate is $\langle c_{i'\sigma'}^\tau P \hat{n}_{I\uparrow} P c_{i\sigma}^\tau \rangle_0$. Let us first take the case of $i \neq I$, $i' \neq I$ and $i \neq i'$, which makes dominant contribution to $V_{k'k}$. After using $P_I \hat{n}_{I\uparrow} P_I = \lambda_{I\uparrow} \hat{n}_{I\uparrow} (1 - \hat{n}_{I\downarrow})$, we take onsite contractions for all the sites except i, i' and I of the numerator neglecting fourth-order terms,

$$\frac{\langle c_{i'\sigma'}^\tau P \hat{n}_{I\uparrow} P c_{i\sigma}^\tau \rangle_0}{\langle P^2 \rangle_0} \approx \frac{\lambda_{I\uparrow} \langle c_{i'\sigma'}^\tau P_i^2 \hat{n}_{I\uparrow} (1 - \hat{n}_{I\downarrow}) P_i^2 c_{i\sigma}^\tau \rangle_0}{\langle P_{i'}^2 \rangle_0 \langle P_I^2 \rangle_0 \langle P_i^2 \rangle_0}. \quad (19)$$

Then, let us work on sites i and i' ,

$$P_i^2 c_{i\sigma}^\dagger = \lambda_{i\sigma} (1 - \hat{n}_{i\bar{\sigma}}) c_{i\sigma}^\dagger, \quad P_i^2 c_{i\sigma} = [(1 - \hat{n}_{i\bar{\sigma}}) + \lambda_{i\bar{\sigma}} \hat{n}_{i\bar{\sigma}}] c_{i\sigma}. \quad (20)$$

For the moment, we take the onsite contractions for $i\bar{\sigma}$ and $i'\bar{\sigma}'$ neglecting intersite contractions between $I \uparrow$ or $I \downarrow$ and them; the terms neglected here are of the third order and will be calculated in the next section. Accordingly, using

$$\frac{\lambda_{i\sigma} (1 - n_{i\bar{\sigma}})}{\langle P_i^2 \rangle_0} = \frac{(1 - n_{i\bar{\sigma}}) + \lambda_{i\bar{\sigma}} n_{i\bar{\sigma}}}{\langle P_i^2 \rangle_0} = 1, \quad (21)$$

(19) can be approximated as

$$\frac{\langle c_{i'\sigma'}^\tau P \hat{n}_{I\uparrow} P c_{i\sigma}^\tau \rangle_0}{\langle P^2 \rangle_0} \approx \frac{\lambda_{I\uparrow} \langle c_{i'\sigma'}^\tau \hat{n}_{I\uparrow} (1 - \hat{n}_{I\downarrow}) c_{i\sigma}^\tau \rangle_0}{\langle P_I^2 \rangle_0}. \quad (22)$$

It is convenient to define mean-value-subtracted operators here,

$$\tilde{n}_{i\sigma} \equiv \hat{n}_{i\sigma} - n_{i\sigma}. \quad (23)$$

Consequently, we obtain

$$\frac{\langle c_{i'\sigma'}^\tau P \tilde{n}_{I\uparrow} P c_{i\sigma}^\tau \rangle_0}{\langle P^2 \rangle_0} \approx \langle c_{i'\sigma'}^\tau \tilde{n}_{I\uparrow} c_{i\sigma}^\tau \rangle_0 - \frac{n_{I\uparrow}}{1 - n_{I\downarrow}} \langle c_{i'\sigma'}^\tau \tilde{n}_{I\downarrow} c_{i\sigma}^\tau \rangle_0. \quad (24)$$

Here, the first term and the second term in the r.h.s. are from the onsite contraction of $1 - \hat{n}_{I\downarrow}$ and $\hat{n}_{I\downarrow}$, respectively; from the residual operators ($\hat{n}_{I\uparrow}$ and $1 - \hat{n}_{I\downarrow}$, respectively), their mean values are subtracted to cancel their onsite contraction.

For the moment, we neglect deviation from (24) for any i and i' , which will be discussed in the next section. Then, it is straightforward to Fourier transform back,

$$\frac{\langle \gamma_{k's} P \tilde{n}_{I\uparrow} P \gamma_{ks}^\dagger \rangle_0}{\langle P^2 \rangle_0} \approx \langle \gamma_{k's} \tilde{n}_{I\uparrow} \gamma_{ks}^\dagger \rangle_0 - \frac{n_{I\uparrow}}{1 - n_{I\downarrow}} \langle \gamma_{k's} \tilde{n}_{I\downarrow} \gamma_{ks}^\dagger \rangle_0. \quad (25)$$

The formula for $\hat{n}_{I\downarrow}$ is obtained by exchanging \uparrow and \downarrow at site I , and these formula represent that $\tilde{n}_{I\sigma}$ is renormalized into $\tilde{n}_{I\sigma} - \tilde{n}_{I\bar{\sigma}} n_{I\sigma} / (1 - n_{I\bar{\sigma}})$.

In fact, the derivation above is valid also for inhomogeneous systems by replacing γ_{ks} with Bogoliubov quasiparticles γ_ℓ . A difference is that the orthogonality of the Gutzwiller-projected Bogoliubov quasiparticle states is only approximately satisfied [7], i.e., errors from the GA can be larger than those in uniform systems. The renormalization of \hat{n}_I in inhomogeneous systems is obtained by summing up $\hat{n}_{I\uparrow}$ and $\hat{n}_{I\downarrow}$ for $\ell \neq \ell'$,

$$\frac{\langle \gamma_{\ell'} P \hat{n}_I P \gamma_\ell^\dagger \rangle_0}{\sqrt{\langle \gamma_{\ell'} P P \gamma_{\ell'}^\dagger \rangle_0 \langle \gamma_\ell P P \gamma_\ell^\dagger \rangle_0}} \approx \left\langle \gamma_{\ell'} \left(g_{I\uparrow}^t \tilde{n}_{I\uparrow} + g_{I\downarrow}^t \tilde{n}_{I\downarrow} \right) \gamma_\ell^\dagger \right\rangle_0, \quad (26)$$

where

$$g_{i\sigma}^t \equiv \frac{1 - n_i}{1 - n_{i\sigma}} \quad (27)$$

is the Gutzwiller renormalization factor for the hopping amplitude.

Returning to our main target, i.e., the non-magnetic uniform system, we can set $g_{I\sigma}^t = g_{I\bar{\sigma}}^t$, then

$$V_{k',k} = \langle k' s | \hat{n}_I | k s \rangle \approx g_{I\sigma}^t (u_{k'} u_k^* - v_{k'} v_k^*) = g_{I\sigma}^t V_{k',k}^{\text{BCS}}, \quad (28)$$

which is exactly the same as the speculation in the previous paper [2] consistent with the numerical results for several k -points by the variational Monte Carlo method, i.e., the renormalization factor is close to g^t and insensitive to model parameters. The important point here may be g^t appears only after summation of up and down spins, $\hat{n}_{I\uparrow} + \hat{n}_{I\downarrow}$, which is a difference from the hopping amplitude renormalization in the real space.

According to the conventional GA [4], what is renormalized is an operator rather than its matrix elements, and thus diagonal and off-diagonal matrix elements have the same renormalization factor. In fact, however, what is renormalized should be matrix elements rather than operators, and diagonal and off-diagonal matrix elements with respect to excited states can have different renormalization factors as demonstrated above.

By exactly the same procedure as above, transition matrix elements between the variational ground state and projected two-quasiparticle excited states can be also calculated. Corresponding to (26),

$$\frac{\langle \Psi_0 | \gamma_\ell \gamma_{\ell'} P \hat{n}_I | \Psi \rangle}{\sqrt{\langle \Psi_0 | \gamma_\ell \gamma_{\ell'} P P \gamma_{\ell'}^\dagger \gamma_\ell^\dagger | \Psi_0 \rangle \langle \Psi | \Psi \rangle}} \approx \langle \Psi_0 | \gamma_\ell \gamma_{\ell'} (g_{I\uparrow}^t \hat{n}_{I\uparrow} + g_{I\downarrow}^t \hat{n}_{I\downarrow}) | \Psi_0 \rangle. \quad (29)$$

4. Corrections to the simple g^t renormalization

In the cases of $i = I \neq i'$, $i' = I \neq i$ and $i = i' = I$, we obtain formulas equivalent to (24). However, for $i = i' \neq I$, we have

$$\frac{\langle c_{i\sigma'}^\tau P \hat{n}_{I\uparrow} P c_{i\sigma}^\tau \rangle_0}{\langle P^2 \rangle_0} \approx \frac{\lambda_{I\uparrow} \langle \hat{n}_{I\uparrow} (1 - \hat{n}_{I\downarrow}) c_{i\sigma'}^\tau P_i^2 c_{i\sigma}^\tau \rangle_0}{\langle P_I^2 \rangle_0 \langle P_i^2 \rangle_0}, \quad (30)$$

where $c_{i\sigma'}^\tau P_i^2 c_{i\sigma}^\tau$ can be explicitly written as

$$c_{i\sigma} P_i^2 c_{i\sigma}^\dagger = \lambda_{i\sigma} (1 - \hat{n}_{i\bar{\sigma}}) (1 - \hat{n}_{i\sigma}), \quad c_{i\sigma}^\dagger P_i^2 c_{i\sigma} = [(1 - \hat{n}_{i\bar{\sigma}}) + \lambda_{i\bar{\sigma}} \hat{n}_{i\bar{\sigma}}] \hat{n}_{i\sigma}, \quad (31)$$

because the other combinations of $c_{i\sigma'}^\tau$ and $c_{i\sigma}^\tau$ yield zero or very small quantities. Then, although the onsite contraction of $i\bar{\sigma}$ with intersite contractions between $i\sigma$ and I yields a formula equivalent to (24), the onsite contraction of $i\sigma$ with intersite contractions between $i\bar{\sigma}$ and I additionally yields the same order of contribution. To compactly write them, let us define

$$\kappa_{i\sigma}^+ \equiv -\frac{1}{1 - n_{i\bar{\sigma}}}, \quad \kappa_{i\sigma}^- \equiv \frac{n_{i\sigma}}{(1 - n_{i\uparrow})(1 - n_{i\downarrow})}, \quad (32)$$

as well as

$$\eta_{i'\sigma', i\sigma} \equiv \langle \hat{n}_{i'\sigma'} \hat{n}_{i\sigma} \rangle_0 - n_{i'\sigma'} n_{i\sigma}, \quad (33)$$

which extracts only intersite contractions in $\langle \hat{n}_{i'\sigma'} \hat{n}_{i\sigma} \rangle_0$. Then, $\langle \hat{n}_{i'\sigma'} (1 - \hat{n}_{i\sigma}) \rangle_0 - n_{i'\sigma'} (1 - n_{i\sigma}) = -\eta_{i'\sigma', i\sigma}$, and $\langle (1 - \hat{n}_{i'\sigma'}) (1 - \hat{n}_{i\sigma}) \rangle_0 - (1 - n_{i'\sigma'}) (1 - n_{i\sigma}) = \eta_{i'\sigma', i\sigma}$. More explicitly,

$$\eta_{i'\sigma, i\sigma} = -\left| \langle c_{i'\sigma}^\dagger c_{i\sigma} \rangle_0 \right|^2, \quad \eta_{i'\bar{\sigma}, i\sigma} = \left| \langle c_{i'\bar{\sigma}}^\dagger c_{i\sigma}^\dagger \rangle_0 \right|^2. \quad (34)$$

Using these notations,

$$\frac{\langle c_{i\sigma}^\tau P \hat{n}_{I\uparrow} P c_{i\sigma}^\tau \rangle_0}{\langle P^2 \rangle_0} \approx \bar{\tau} \left(\eta_{I\uparrow, i\sigma} - \frac{n_{I\uparrow}}{1 - n_{I\downarrow}} \eta_{I\downarrow, i\sigma} \right) + \kappa_{i\sigma}^\tau \langle c_{i\sigma}^\tau c_{i\sigma}^\tau \rangle_0 \left(\eta_{I\uparrow, i\bar{\sigma}} - \frac{n_{I\uparrow}}{1 - n_{I\downarrow}} \eta_{I\downarrow, i\bar{\sigma}} \right). \quad (35)$$

By summing up $\hat{n}_{I\uparrow}$ and $\hat{n}_{I\downarrow}$,

$$\frac{\langle c_{i\sigma}^\tau P(\tilde{n}_{I\uparrow} + \tilde{n}_{I\downarrow}) P c_{i\sigma}^\tau \rangle_0}{\langle P^2 \rangle_0} \approx \bar{\tau} (g_{I\uparrow}^t \eta_{I\uparrow, i\sigma} + g_{I\downarrow}^t \eta_{I\downarrow, i\sigma}) + \kappa_{i\sigma}^\tau \langle c_{i\sigma}^\tau c_{i\sigma}^\tau \rangle_0 (g_{I\uparrow}^t \eta_{I\uparrow, i\bar{\sigma}} + g_{I\downarrow}^t \eta_{I\downarrow, i\bar{\sigma}}). \quad (36)$$

Since $i \neq i'$ occurs more often than $i = i'$, the third-order terms neglected in the previous section for the case of $i \neq I$, $i' \neq I$, and $i \neq i'$ may have larger contribution than the newly derived terms above. Such terms are derived by taking into account intersite contraction including $i\bar{\sigma}$ and $i'\bar{\sigma}'$. However, if intersite contractions are taken between $i\bar{\sigma}$ and $i'\bar{\sigma}'$ and the onsite contractions are taken for I , then such terms do not contribute as explained around (18). Using the notation above, (20) is rewritten as

$$\frac{P_i^2 c_{i\sigma}^\tau}{\langle P_i^2 \rangle_0} = (1 + \kappa_{i\sigma}^\tau \tilde{n}_{i\bar{\sigma}}) c_{i\sigma}^\tau. \quad (37)$$

Then, for $\tau' = -\tau\sigma\sigma'$ (\uparrow, \downarrow and $+1, -1$ are used interchangeably),

$$\begin{aligned} \frac{\langle c_{i'\sigma'}^{\tau'} P(\tilde{n}_{I\uparrow} + \tilde{n}_{I\downarrow}) P c_{i'\sigma'}^{\tau'} \rangle_0}{\langle P^2 \rangle_0} &\approx g_{I\uparrow}^t \langle c_{i'\sigma'}^{\tau'} \tilde{n}_{I\uparrow} c_{i'\sigma'}^{\tau'} \rangle_0 + g_{I\downarrow}^t \langle c_{i'\sigma'}^{\tau'} \tilde{n}_{I\downarrow} c_{i'\sigma'}^{\tau'} \rangle_0 \\ &+ \langle c_{i'\sigma'}^{\tau'} c_{i\sigma}^\tau \rangle_0 \left[\kappa_{i\sigma}^\tau (g_{I\uparrow}^t \eta_{I\uparrow, i\bar{\sigma}} + g_{I\downarrow}^t \eta_{I\downarrow, i\bar{\sigma}}) + \kappa_{i'\sigma'}^{\tau'} (g_{I\uparrow}^t \eta_{I\uparrow, i'\bar{\sigma}'} + g_{I\downarrow}^t \eta_{I\downarrow, i'\bar{\sigma}'} \right] \\ &+ \sigma \kappa_{i\sigma}^\tau \langle c_{i'\sigma'}^{\tau'} c_{i\bar{\sigma}}^\tau \rangle_0 (g_{I\uparrow}^t \langle c_{I\uparrow}^\dagger c_{i\bar{\sigma}}^\tau \rangle_0 \langle c_{I\uparrow} c_{i\tau}^\tau \rangle_0 - g_{I\downarrow}^t \langle c_{I\downarrow}^\dagger c_{i\bar{\sigma}}^\tau \rangle_0 \langle c_{I\downarrow} c_{i\tau}^\tau \rangle_0) \\ &+ \sigma' \kappa_{i'\sigma'}^{\tau'} \langle c_{i'\sigma'}^{\tau'} c_{i\sigma}^\tau \rangle_0 (g_{I\uparrow}^t \langle c_{I\uparrow}^\dagger c_{i'\bar{\sigma}'}^{\tau'} \rangle_0 \langle c_{I\uparrow} c_{i'\tau'}^{\tau'} \rangle_0 - g_{I\downarrow}^t \langle c_{I\downarrow}^\dagger c_{i'\bar{\sigma}'}^{\tau'} \rangle_0 \langle c_{I\downarrow} c_{i'\tau'}^{\tau'} \rangle_0). \end{aligned} \quad (38)$$

Although all the new terms in (36) and (38) contain the g^t factors, they are not so simple as (24) and inhibit the straightforward analytical transform back to k -representation. In other words, they cause k -dependence of the renormalization. Since the ratio between the leading order and the corrections calculated in (38) is only of the first order, the influence from the corrections may be larger than those in the GA for the real-space hopping amplitude, where the ratio is of the second order.

Other corrections are the terms neglected in (15). We expect that they only slightly change the magnitude of the leading order, and that their contribution is probably not very important.

5. General estimation of higher-order terms

Let us estimate the other higher-order terms neglected above. The terms appearing in the Wick expansion can be classified into three groups by how to take contractions of $\hat{n}_{I\sigma}(1 - \hat{n}_{I\bar{\sigma}})$: (i) Onsite contractions are taken both for $I \uparrow$ and $I \downarrow$. These terms do not contribute to $V_{k'k}$ as explained around (18). (ii) If intersite contractions are taken for $I\sigma$ and the onsite contraction is taken for $I\bar{\sigma}$, then $\lambda_{I\sigma} \hat{n}_{I\sigma}(1 - \hat{n}_{I\bar{\sigma}})/\langle P_I^2 \rangle_0$ is reduced to $\tilde{n}_{I\sigma}$. Doing the same for $\lambda_{I\bar{\sigma}} \hat{n}_{I\bar{\sigma}}(1 - \hat{n}_{I\sigma})/\langle P_I^2 \rangle_0$ yields $-\tilde{n}_{I\sigma} n_{I\bar{\sigma}}/(1 - n_{I\sigma})$. Then their summation is $g_{I\sigma}^t \tilde{n}_{I\sigma}$. Namely, all of these terms are proportional to $g_{I\sigma}^t$. (iii) For the other terms, intersite contractions are taken both for $I \uparrow$ and $I \downarrow$. Naive evaluation of these terms does not yield any explicit factor vanishing at half filling, and we expect that many terms cancel out each other in some way. Instead, to derive explicit

renormalization, let us consider such contractions for $\langle k's|(1 - \hat{n}_{I\uparrow})(1 - \hat{n}_{I\downarrow})|ks\rangle$, which is equivalent to $V_{k',k}$ for $k \neq k'$. Then we can replace as

$$\frac{(1 - \hat{n}_{I\uparrow})(1 - \hat{n}_{I\downarrow})}{\langle P_I^2 \rangle_0} \Rightarrow \frac{1 - n_I}{(1 - n_{I\uparrow})(1 - n_{I\downarrow})} \tilde{n}_{I\uparrow} \tilde{n}_{I\downarrow}, \quad (39)$$

i.e., all such terms contain $g_{I\sigma}^t/(1 - n_{I\bar{\sigma}})$ explicitly. These considerations in (i), (ii) and (iii) above demonstrate that $V_{k',k}$ contains overall factor $g_{I\sigma}^t$.

6. Magnetic impurity renormalization

Let us consider a simple magnetic impurity (4), i.e., local magnetic field is applied at site I . Its renormalization can be easily calculated by subtraction instead of summation of renormalized $\hat{n}_{I\uparrow}$ and $\hat{n}_{I\downarrow}$ using formulas above. Corresponding to (26) and (28),

$$\frac{\langle \gamma_{\ell'} P S_I^z P \gamma_{\ell} \rangle_0}{\sqrt{\langle \gamma_{\ell'} P^2 \gamma_{\ell'} \rangle_0 \langle \gamma_{\ell} P^2 \gamma_{\ell} \rangle_0}} \approx \frac{1}{2} \left[\frac{1 - n_{I\uparrow} + n_{I\downarrow}}{1 - n_{I\uparrow}} \langle \gamma_{\ell'} \tilde{n}_{I\uparrow} \gamma_{\ell}^{\dagger} \rangle_0 - \frac{1 - n_{I\downarrow} + n_{I\uparrow}}{1 - n_{I\downarrow}} \langle \gamma_{\ell'} \tilde{n}_{I\downarrow} \gamma_{\ell}^{\dagger} \rangle_0 \right] \quad (40)$$

$$\longrightarrow \frac{1}{1 - n_{I\sigma}} \langle \gamma_{\ell'} S_I^z \gamma_{\ell}^{\dagger} \rangle_0 \quad (n_{\uparrow} = n_{\downarrow}), \quad (41)$$

The renormalization factor for $n_{I\uparrow} = n_{I\downarrow}$ is $(1 - n_{I\sigma})^{-1}$, which is the square root of the Gutzwiller renormalization factor for the exchange interaction. Namely, in contrast to the non-magnetic impurity, the magnetic impurity is strengthened by the strong electron correlation. It also makes a good contrast with the unrenormalized diagonal matrix element $\langle S_I^z \rangle = \langle S_I^z \rangle_0$ (to derive this, the limit of $\lambda_{I\uparrow} - \lambda_{I\downarrow} \rightarrow 0$ should be taken at the end starting from $\lambda_{I\uparrow} \neq \lambda_{I\downarrow}$).

In fact, also for magnetic systems ($n_{I\uparrow} \neq n_{I\downarrow}$), the factors appearing in (40) are equivalent to those in the renormalization of the exchange interaction derived in [7], i.e.,

$$\langle S_i^z S_j^z \rangle \approx \langle S_i^z \rangle_0 \langle S_j^z \rangle_0 + \frac{1}{4} \sum_{\sigma, \sigma'} \eta_{i\sigma, j\sigma'} \left(\sigma \frac{1 - 2\sigma \langle S_i^z \rangle_0}{1 - n_{i\sigma}} \right) \left(\sigma' \frac{1 - 2\sigma' \langle S_j^z \rangle_0}{1 - n_{j\sigma'}} \right). \quad (42)$$

Although it is not explicitly noted in [7], in this renormalization of the spin interaction, the first term is from onsite contractions and not renormalized (from diagonal matrix elements of the spin- z operators), whereas the second term including intersite contractions is enhanced by the renormalization factor (from the second order of the transition matrix elements of the spin- z operators). In fact, as shown in the next section, charge interaction is also renormalized in a similar manner although the direction of renormalization is opposite.

7. Charge interaction renormalization

The conventional GA [4] relates $\langle \hat{O} \rangle$ to $\langle \hat{O} \rangle_0$ for an operator \hat{O} using a renormalization factor. By following this procedure, the renormalization factor is unity for the charge interaction, namely,

$$\langle \hat{n}_i \hat{n}_j \rangle \stackrel{?}{\approx} \langle \hat{n}_i \hat{n}_j \rangle_0 = n_i n_j + \sum_{\sigma, \sigma'} \eta_{i\sigma, j\sigma'} \quad (43)$$

However, this approximation is correct only for the leading term $n_i n_j$ and the renormalization factor is likely to be derived by taking only the lowest order into account. Using a procedure similar to that for the non-magnetic impurity, more careful analysis can be carried out, i.e.,

$$\begin{aligned}
\langle \hat{n}_i \hat{n}_j \rangle &\approx \sum_{\sigma, \sigma'} \lambda_{i\sigma} \lambda_{j\sigma'} \frac{\langle \hat{n}_{i\sigma} (1 - \hat{n}_{i\bar{\sigma}}) \hat{n}_{j\sigma'} (1 - \hat{n}_{j\bar{\sigma}'}) \rangle_0}{\langle P_i \rangle_0 \langle P_j \rangle_0} \\
&\approx n_i n_j + \sum_{\sigma, \sigma'} \left(\eta_{i\sigma, j\sigma'} - \frac{n_{i\sigma}}{1 - n_{i\bar{\sigma}}} \eta_{i\bar{\sigma}, j\sigma'} - \frac{n_{j\sigma'}}{1 - n_{j\bar{\sigma}'}} \eta_{i\sigma, j\bar{\sigma}'} + \frac{n_{i\sigma}}{1 - n_{i\bar{\sigma}}} \frac{n_{j\sigma'}}{1 - n_{j\bar{\sigma}'}} \eta_{i\bar{\sigma}, j\bar{\sigma}'} \right) \\
&= n_i n_j + \sum_{\sigma, \sigma'} g_{i\sigma}^t g_{j\sigma'}^t \eta_{i\sigma, j\sigma'}. \tag{44}
\end{aligned}$$

At the half filling, any state is an eigenstate of $\hat{n}_i \hat{n}_j$ with the eigenvalue unity by definition because every site is occupied by one electron and there is no particle number fluctuation, which contradicts (43) but is consistent with (44). In fact, the second term of r.h.s. of (44) is the second order of (29), namely, it comes from a process in which \hat{n}_j creates two quasiparticles and \hat{n}_i annihilates them.

To our knowledge, every calculation in the literature on the GA is using (43) instead of (44) including the calculation by the author himself, and probably this error is pointed out for the first time here. However, this charge interaction usually does not give very important contribution in t - J -type models, and this correction is likely to make only minor modification to numerical values. Therefore, we expect that main conclusions are not drastically changed by this correction. Following this correction, equations in [7] should be modified, namely, $(3g_{ij}^s - 1)$ and $(3g_{ij}^s + 1)$ in (14) and (15) should be replaced by $(3g_{ij}^s - g_{ii}^t g_{jj}^t)$ and $(3g_{ij}^s + g_{ii}^t g_{jj}^t)$, respectively, and derivative of g_{ii}^t should be also considered for (16).

8. Conclusion

Since the Gutzwiller approximation is formulated to (almost) conserve the particle number at the Gutzwiller projection, one may consider that quantities related to particle number operators are not renormalized. However, since the particle number is an expectation value with respect to an assumed ground state, the constraint of its conservation does not restrict transition matrix elements with excited states. Our results here correct description by the conventional Gutzwiller approximation in the literature, where such renormalization factors are calculated with a focus on diagonal matrix elements or lowest-order terms and regarded as unity. The results in this paper are general and do not depend on parameters. Namely, they are valid both for attractive and repulsive impurity potentials and both for attractive and repulsive charge interactions.

The Fourier-transformed impurity potential has a form of hopping in the k -space. We have derived similarities and differences between this “hopping” in the k -space and in the real space under real-space electron double-occupancy prohibition. As a similarity, they are strongly renormalized to decrease with hole concentration x , and

their renormalization factor is $g^t = 2x/(1+x)$ in uniform non-magnetic systems. In addition, the higher order terms also contain g^t . It should represent that not many available seats to hop are left because of the electron repulsion. A difference is, however, $\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle$ of each σ is renormalized in the real space, whereas renormalization of $\sum_\sigma \langle c_{k'\sigma}^\dagger c_{k\sigma} \rangle$ appears only after the summation over spin $\sigma = \pm$ in the k -space. If this summation is replaced by subtraction, which corresponds to a magnetic impurity in the real space, then the direction of the renormalization is reversed, i.e., the renormalization factor is larger than unity and equivalent to the square root of that for the exchange interaction. As another difference, the corrections to the leading order term in the k -space can be larger and have more complicated expression than those in the real space.

As related calculation, renormalization of charge interaction has been also derived. The leading order is rather trivial and unrenormalized, i.e., it is the product of particle densities at the two relevant sites. The next leading order term is the second order of transition matrix elements of the number operators with excited states. Since the transition matrix elements are renormalized by g^t , these second order terms are renormalized by $(g^t)^2$, namely, strongly reduced. These terms include hopping and pairing amplitude and are relevant to the mean-field approximation. Similar relation is found also in the z -component of the exchange interaction. Namely, the leading order is the product of spin- z densities at the two relevant sites. The next term is the second order of transition matrix elements of the spin- z operator, which is strengthened by the electron repulsion. At the half filling, any state is an eigenstate of $\hat{n}_i \hat{n}_j$, with the eigenvalue unity. In fact, (44) satisfies it even in magnetic systems, which may demonstrate that the choice of fugacity factors by (9) is reasonable. Other choices of fugacity factors also discussed in [7] do not seem to satisfy it in magnetic systems, and their use is likely to be restricted in systems with small magnetic moments.

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